CHBE 505
Advanced Numerical Methods

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Office: B235 Abercrombie
Class Room: HRZ 211

Class Hours: 9:25 AM –10:40 AM (T, Th)
Office Hours: By Appointment
TA hours: TBD

Teaching assistants

[provisionally] Arjun Valiya Parambathu (av42@rice.edu)

Course Description

Modern engineering practice and scientific research is increasingly reliant on scientific computing, and scientific computing is founded on numerical methods. In this course, we will focus on the mathematics underlying numerical methods and their efficient computer implementation. Scientific computing necessarily requires proficiency in a programming language. We will use the Python language in this course, as it is a well-established programming language that is welcoming to newcomers. It is extensively used in scientific computing (both in academia and in industry) and is excellent for quickly prototyping ideas. Becoming familiar with the Spyder IDE (Integrated Development Environment), Jupyter notebook, Matplotlib graphing package, and extensive libraries for high performance computing will help the student learn vital skills that the student can translate to their work in other courses, in research, or work outside graduate school.

Course Objectives

The course objectives are to ensure students are (a) proficient in the mathematics underlying core numerical methods and (b) be able to make sense of and use computational techniques in their work. We plan to cover the following topics.

1. Linear Algebraic Systems
2. Nonlinear Algebraic Systems
3. Initial Value Problems
4. Boundary Value Problems

5. Probability Theory, Stochastic Methods, and Basic Ideas in Data Analysis
6. Numerical Optimization (if time permits)
7. Fourier Methods (if time permits)

Required Textbook

- *Computational Physics* by Mark Newman
  - This is an undergraduate level text, but is also suitable for a beginning graduate student. I like the text because of its reliance on Python and emphasis on physics. We will supplement the development in this text with our course notes.
  - For topics not in this text, we will rely on our course notes.
- If you have a personal laptop (highly recommended), please install the freely available Anaconda distribution of Python.

Supplemental Reading

- *Numerical Methods with Chemical Engineering Applications* by Kevin Dorfman and Prodromos Daoutidis
  - We used this text last year. This is an excellent text and could prove helpful for supplementary reading. Text relies on MATLAB.
- *Numerical Recipes: The art of scientific computing* by Press, Teukolsky, Vellerling, and Flannery.
  - This *fantastic book* provides an exhaustive tour of basic and advanced numerical methods. The implementation of methods is discussed in detail and code is provided for different languages, such as Fortran and C. This is a *must have* book for any researcher / engineer who expects to do extensive numerical work.
- Class Notes
  - Class notes will be posted on Canvas.

Course Organization

- The course will comprise six or seven assignments. Some of these will be designated as non-pledged and others as pledged. (See Honor code policy below.)
- We will have a final project. The student (in a group of no more than two) will study and implement a numerical method in the context of a physical application. The project will involve running calculations, preparing a report, and a presentation before the entire class.

Honor code Policy

Students are encouraged to talk to each other, the teaching assistants, the instructor, or anyone else about any assignment in the course that is not specifically designated as pledged. For assignments that are pledged, you can **only discuss with the instructor and/or TAs**; you cannot consult any other resource (excluding programming language specific help files). For all assignments, consulting another student's solution is prohibited. Your submissions should not be copied from any source.

ADA Statement

Any student with a documented disability needing academic adjustments or accommodations is requested to speak with the instructor during the **first two weeks of class**. All discussions will remain confidential. Students with disabilities will need to also contact Disability Support Services in the Allen Center.

Grading Policy

Grade	%
Assignments	65
Project	30
Attendance	5

Late assignments will incur a penalty of 20% / day after the submission deadline. Provisionally, we plan to follow the distribution below in assigning letter grades. Reasonable adjustments will be made based on how the course evolves.

Grade	%
A+	≥ 98
A	$92.0 - 97.9$
A-	$86.0 - 91.9$
B+	$80.0 - 85.9$
B	$70.0 - 79.9$
B-	$60.0 - 69.9$
C	< 59.9